1,3-Propanediol, diacetate
628-66-0 | DTXSID30211889

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 206 °C

Global applicability domain: Inside

Local applicability domain index: 1.00

Confidence level: 8.71e-01

Nearest Neighbors from the Training Set

Image not found
Diethyl propanedioate
Measured: 200
Predicted: 206

Image not found
Butanedioic acid, ethyl methyl ester
Measured: 208
Predicted: 206

Image not found
1,3-Propanediol, diacetate
Measured: 210
Predicted: 206

Image not found
Dimethyl glutarate
Measured: 214
Predicted: 206

Image not found
Propylene glycol diacetate
Measured: 191
Predicted: 198